# FINE SPLITTING OF ENERGY LEVELS IN MANY-ELECTRON ATOMS AND IONS

*O.B. Nadykto, B.A. Nadykto*

RFNC-VNIIEF, Arzamas-16 (Sarov), Nizhni Novgorod region, 607190,
E-mail:nadykto@vniief.ru, Fax: 83130 45772

Ref. [1] suggests trial radial wave functions for one-electron ions in the form of the product of one-electron functions

$$R_{nl} = -\left(\frac{(n-l-1)!}{((n+l)!)^3 2n}\right)^{1/2}\left(\frac{2n}{x}\right)^{3/2} e^{-\frac{nr}{x}}\left(\frac{2nr}{x}\right)^{l} L_{n+l}^{2l+1}(2nr/x)\,. \qquad (1)$$

It is well known that in the relativistic approximation hydrogen-like ion energies are described by Dirac-Sommerfeld relation:

$$E(Z,n,k) = mc^2\left[\left[1+\left[\frac{\alpha Z}{n-k+(k^2-\alpha^2 Z^2)^{1/2}}\right]^2\right]^{-1/2} - 1\right] \qquad (2)$$

where $n$ is the principal quantum number, $k= j+1/2$, $j$ is the quantum number of net moment (the sum of orbital moment and spin), α is the fine structure constant, $m$ is electron mass, $c$ is light velocity, $Z$ is ion nuclear charge. For $k=n$ ($j = n - 1/2$)

In the semiempirical approach [2], when calculating energy of many-electron ions, not only Coulomb interaction, but also additional interaction between electrons from different shells, which depends on orbital quantum number $l$, is taken into account. In so doing the electron wave function parameter changes noticeably. The energy of states (both the ground state and excited states) of the outer electron of lithium-like ions is described in most cases with an accuracy better than $10^{-4}$. When the energy description has been obtained, calculated fine splitting (7) agrees with the experimental value with an accuracy of ~1% or better without using any additional empirical parameters.

The distance between the extreme components of the triplet of states $1s^22pns\ ^3P_2 - {}^3P_0$ is very close to the splitting of states $1s^22p\ ^3P_{3/2} - {}^3P_{1/2}$ of lithium-like ions, that is this is the difference between energies of states $1s^22p(^3P_{3/2})ns - 1s^22p(^3P_{1/2})ns$. Attraction by the outer ns shell increases the wave function parameter of 2p electron as compared to state $1s^22p$, which leads to a decrease in its fine splitting. With increasing n the fine splitting of states $1s^22pns\ ^3P_2 - {}^3P_0$ increases and approaches the value for states $1s^22p$. The distance between the extreme components of the triplet of states $1s^22p^2(^3P)ns\ ^4P$ is close to the difference between energies of states $1s^22p^2\ ^3P_2 - {}^3P_0$. Parameters of interaction of electrons in configurations $1s^22s2pnl$ of boron-like ions had been selected, which were used in the calculations of multiply charged ion characteristics. The calculated intervals of fine splitting make a certain portion of interval $1s^22s2p\ ^3P_2$ - $1s^22s2p\ ^3P_0$ of beryllium-like ions, which changes slightly due to interaction of 2s2p electrons with outer nl electrons. The unusual behavior of the fine splitting with n can serve a distinctive feature of these states.

Energy required for knockout of electrons from inner shells of neutral atoms is significantly less (by up to 25%) than energy of ionization of ion, which outer electrons are removed in. This does not means a smaller bond of knocked-out electron in neutral atom. In this case, when inner electron knockout takes place, bond energy of outer electrons in the final state increases due to increase in the charge acting on them by one. The final-state fine splitting depends mainly on energy of remaining inner electrons rather than on transition energy. The transition energy depends on aggregative or chemical state of material, i.e. on what the state of the outer electron shell is which the knocked-out inner electron has been brought into. The fine splitting of energy of inner states is essentially independent of these changes. The fine splitting is smaller significantly for the states of outer electrons than for inner electrons.

References

1. B.A. Nadykto // VANT. Ser. Teoreticheskaya i Prikladnaya Fizika. 1994. Issue 1. P. 32
2. B.A. Nadykto // UFN. 1993. V. 163, No. 9. P. 37-75.